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Efficient prediction of (p,n) yields

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Efficient prediction of (p,n) yields

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In the continuous deceleration approximation, charged particles decelerate without any spread in energy as they traverse matter. This approximation simplifies the calculation of the yield of nuclear reactions, for which the cross-section depends on the particle energy. We calculated (p,n) yields for a LiF target, using the Bethe-Bloch relation for proton deceleration, and predicted that the maximum yield would be around 0.25% neutrons per incident proton, for an initial proton energy of 70 MeV or higher. Yield-energy relations calculated in this way can readily be used to optimize source and (p,n) converter characteristics.

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I. INTRODUCTION

Nuclear reactions are used increasingly in science and technology, including novel sources employing, for example, laser-accelerated particles. Detailed design calculations are usually performed using computer programs to simulate the reactions with explicit spatial and spectral resolution. Although such simulations are in principle the most accurate method of calculation, it can be inconvenient and inefficient to optimize design parameters, and there is less scope to obtain physical insights into the processes and their optimzation. Moreover, it is highly desirable to use alternative methods for performing any calculation which may have safety implications.

We are developing sources of pulsed neutrons, using laser-accelerated protons and (p,n) reactions in a converter material. An important measure of the performance of such sources is the neutron yield, which captures the efficiency of a given configuration in a compact form, and is also useful in the assessment of radiation doses. Here we describe a method of calculating neutron yields reasonably directly and efficiently, without requiring large-scale simulation programs.

II. NEUTRON YIELD FROM MONOENERGETIC PROTONS

Consider a beam of protons interacting with a target in which (p,n) reactions can occur. As the protons traverse the target, they lose kinetic energy. In reality, individual protons undergo quantized scattering interactions with electrons and nuclei in the target, and a spectrum of energies and directions is produced from incident protons of a given energy. However, on scales large compared with the interatomic spacing, the deceleration is represented accurately by the continuous deceleration approximation (CDA), giving an energy loss dE/dx which is a function of the proton energy E. In this approximation, initially monoenergetic protons all decelerate at the same rate, so the distribution of their energies does not broaden as they pass through the target. Although the beam divergence increases with propagation distance through the target, most of this divergence occurs at the lowest speeds. Ignoring divergence, the CDA thus means that a unique kinetic energy is associated with each position x through the target.

Given an expression for

$$-\frac{dE}{dx} \equiv f_s(E), \tag{1}$$

it can be integrated to obtain

$$x(E) = -\int_{E_0}^{E} \frac{dE'}{f_s(E')} \tag{2}$$

and inverted to obtain $E(x)$. Convenient expressions may be obtained by redefining position with respect to the point at which the protons come to rest, $E = 0$. The deceleration function f_s becomes more complicated at low energies, so we choose instead the point at which the protons slow to some minimum energy, $E_{\rm min}$. $E_{\rm min}$ could be either the energy at which the deceleration model breaks down, or a representative energy below which no (p,n) reactions can take place. We choose to orient the position axis in the direction the protons come *from*. In terms of this position $X \equiv x(E_{\rm min}) - x$,

$$X(E) = \int_{E_{\rm min}}^{E} \frac{dE'}{f_s(E')}, \tag{3}$$

which is a universal curve for a given target material (and beam ion, as it applies to other particles than protons), irrespective of the energy of the incident particles,

E_0. Different values of E_0 correspond to different initial values of X. We followed a similar procedure when calculating algebraic solutions for particle range calculated using the Bethe equation [1].

Protons are removed by reaction, so the number N varies with position according to the reaction cross-section σ and number density ρ of target nuclei available for a given reaction,

$$\frac{1}{N}\frac{dN}{dx} = -\sum_i \rho_i \sigma_i(E), \tag{4}$$

so

$$\begin{aligned} N(x) &= N_0 \exp\left\{-\int_0^x \sum_i \rho_i\sigma_i[E(x')]\,dx'\right\}, &(5)\\ N(X) &= N_f \exp\left\{\int_0^X \sum_i \rho_i\sigma_i[E(X')]\,dX'\right\}, &(6)\\ &= N_0 \exp\left\{-\int_0^X \sum_i \rho_i\sigma_i[E(X')]\,dX'\right\}, &(7)\end{aligned}$$

where N_0 is the number of incident protons and N_f the number reaching E_{min} without reacting. If the deceleration of the protons is non-zero, the integral can be calculated with respect to energy instead of position:

$$\begin{aligned} N &= N_0 \exp\left[-\int_{E_{\mathrm{min}}}^{E_0} \frac{1}{f_s(E')}\sum_i \rho_i\sigma_i(E')\,dE'\right] &(8)\\ &= N_f \exp\left[\int_{E_{\mathrm{min}}}^{E_0} \frac{1}{f_s(E')}\sum_i \rho_i\sigma_i(E')\,dE'\right]. &(9)\end{aligned}$$

These expressions are convenient in that the range $X(E)$ need not be calculated explicitly or inverted to find $E(x)$, though the integral cannot be evaluated as a general, algebraic solution as it depends on the form of the $\sigma_i(E)$.

The production of neutrons (cumulative number N_n) is given by

$$\frac{1}{N}\frac{dN_n}{dx} = \sum_i N_i \rho_i \sigma_i(E) \tag{10}$$

where N_i is the number of neutrons produced by reaction i. For (p,n) reactions ($N_i = 1$) with no competing processes to remove protons,

$$N_n(x) = N_0 - N(x). \tag{11}$$

The calculations above do not give the neutron spectrum, just the overall number of neutrons produced. The formulations in terms of X or E are suited to determining the maximum neutron yield, implying a minimum converter thickness for the highest-energy protons to decelerate to E_{min}. The formulations in terms of x are suited to calculating the neutron yield for a given converter thickness.

TABLE I: Isotopes in LiF.

isotope	**abundance** (at. %)
^{7}Li	92.5
^{6}Li	7.5
^{19}F	100

TABLE II: (p,n) reaction energetics in LiF.

isotope	**energy released, Q** (MeV)	**CM threshold energy** (MeV)	**proton threshold energy** (MeV)
^{7}Li	-1.644	1.880	2.456
^{6}Li	-5.071	5.920	8.058
^{19}F	-4.021	4.234	4.691

III. POLYENERGETIC PROTONS

For a spectrum of incident protons $n_0(E)$, the calculations above can simply be performed for a set of discrete energies representing the spectrum, then integrated with weighting according to the amplitude in the spectrum. The relations in terms of X above are less useful, since the absolute location of the origin $X = 0$ varies with E.

IV. APPLICATION TO LIF

LiF is a convenient (p,n) converter material as it is readily available, has low cost, is conveniently in solid form, and is relatively non-hazardous. Li occurs in two stable isotopes of atomic weight 6 and 7. The relative abundance depends on the source of the Li; for the present study we assumed average terrestrial abundances (Table I). Both isotopes of Li undergo (p,n) reactions, though ^{6}Li has a significantly higher threshold energy. ^{19}F, the only stable isotope, also undergoes (p,n) reactions, though with a higher threshold energy than for ^{7}Li. The mass density of LiF is 2.638 g/cm^3 [2], so the density of both Li and F atoms is 6.11×10^{28}/m^3.

Energetics for the (p,n) reactions were taken from the Atomic Mass Data Center [3] (Table II). Reaction cross-section data were taken from the ENDF library [4]. For ^{7}Li, (p,n) cross-sections have been measured in detail up to ∼4 MeV, and with successively coarser energy resolution up to ∼25 and ∼200 MeV. For ^{6}Li, no (p,n) cross-sections were reported; the interaction is more likely to result in ^{3}He and ^{4}He being produced. For ^{19}F, (p,n) cross-sections have been measured in detail up to ∼7 MeV, and sparsely up to ∼30 MeV. (Figs 1 and 2).

The Bethe equation [5] describes the deceleration of charged particles by interaction with the electrons in

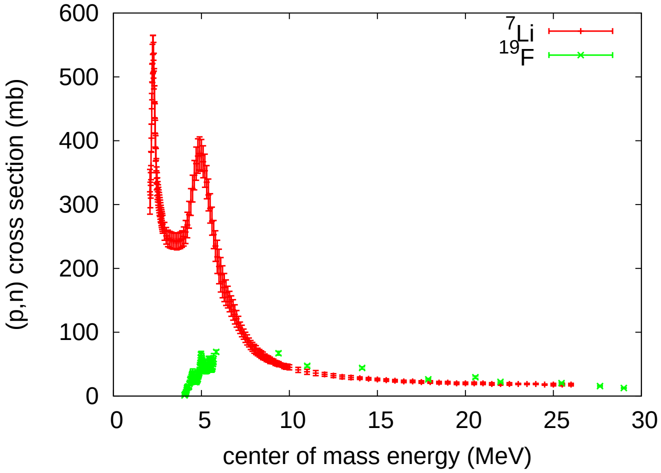

FIG. 1: (p,n) cross-sections for ^{7}Li and ^{19}F.

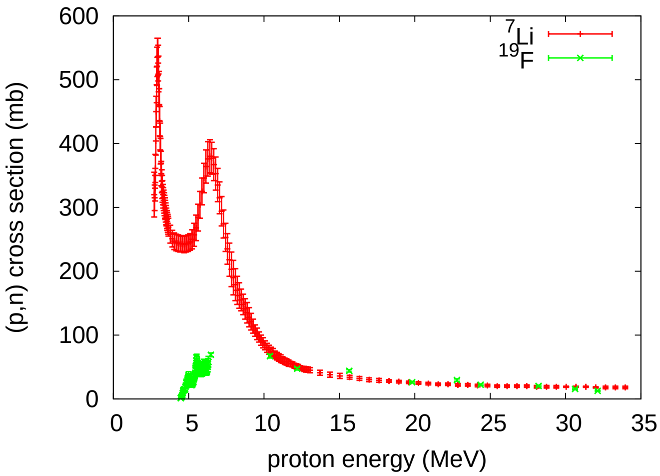

FIG. 2: (p,n) cross-sections for ^{7}Li and ^{19}F, plotted with respect to proton energy for target nuclei at rest.

matter:

$$f_s(E) = \frac{4\pi}{m_e c^2}\frac{NZz^2}{\beta^2}\left(\frac{q^2}{4\pi\epsilon_0}\right)^2\left[\ln\frac{2m_e c^2\beta^2}{\bar{I}\,(1-\beta^2)} - \beta^2\right] \tag{12}$$

where $\beta = v/c$, v is the ion speed, $\bar{I}$ is the effective ionization of the target material, Z and z are the atomic numbers of the target and ion species respectively, N is the number density of target nuclei, m_e is the mass of an electron, ϵ_0 is the permittivity of free space, and c is the speed of light. The Bethe relation holds for elements, and should be $\sim$1% accurate in the regime of interest. The stopping power of Li and F together was calculated using the Bragg additive estimate,

$$f_s(E) = \sum_i f_s(N_i, Z_i, E). \tag{13}$$

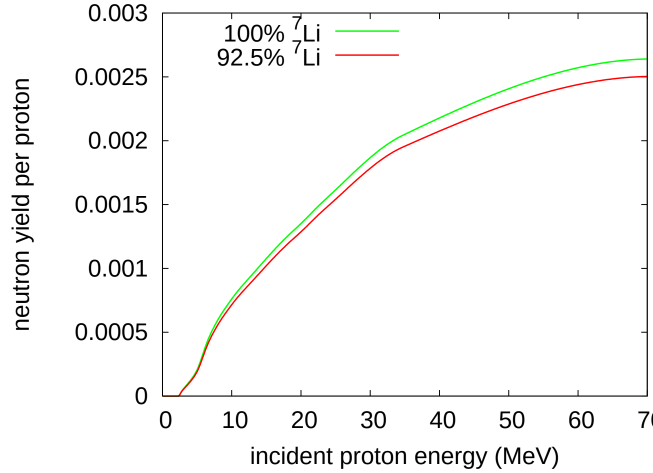

FIG. 3: Neutron yield predicted from (p,n) reaction in a LiF target.

For each target specie, the Bloch estimate [6] was used for its ionization,

$$\bar{I} \simeq 10Zq, \tag{14}$$

where Z is the atomic number of the specie.

The integration in Eq. 9 was evaluated numerically using adaptive-stepsize algorithms, and the exponent calculated for a series of increasing values of the energy E. It was necessary to extrapolate the (p,n) cross-sections beyond the range of their measurements. The cross-section for each element was modeled as decreasing linearly to zero, at a center-of-mass energy of 62 MeV for ^{7}Li and 33 MeV for ^{19}F. These choices of energy were evident as inflections in the calculated yield. Yields were calculated for a target in which the Li was 100% ^{7}Li, and also for the natural abundance by scaling down the cross-section. Up to 0.25% of the protons were predicted to take part in (p,n) reactions, and the yield was predicted to increase steadily up to an incident proton energy of 70.8 MeV, corresponding to the cutoff in ^{7}Li cross-section at 62 MeV (Fig. 3). The yield was calculated to increase most rapidly with energy near the peak of the ^{7}Li (p,n) cross-section. The calculated yield is consistent with our previous calculations using a numerical integration of the proton spectrum with position through the target [7]. These yield calculations assume that the target is thick enough to decelerate the protons through the full range of energies for the (p,n) reactions to occur, i.e. to below 2.456 MeV. The thickness of LiF necessary was calculated from the proton range [1] and also by numerical integration of Eq. 3, giving almost identical results (Fig.4).

In laser acceleration of ions, a common figure of merit is the efficiency of converting laser energy to ion energy. When it is desired to then use the laser-accelerated ions in nuclear reactions, the ion yield is also important. Energy-yield relations calculated as described above can

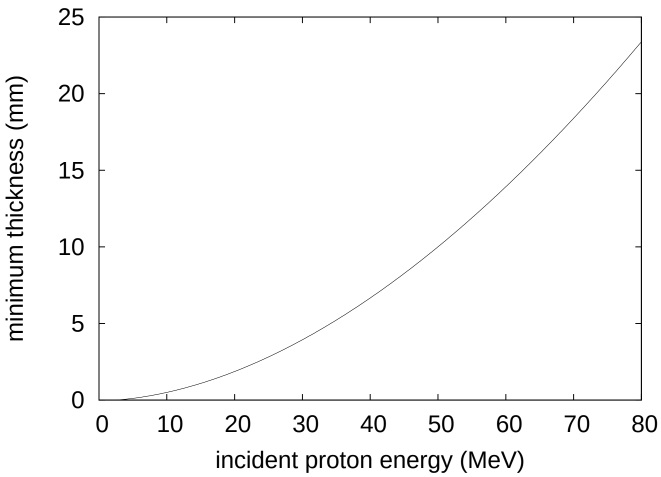

FIG. 4: Thickness of LiF necessary for maximum production of neutrons.

be used directly to trade off energy efficiency against particle yield, allowing daughter-particle sources to be optimized more efficiently.

V. CONCLUSIONS

Compact expressions were developed to relate the yield of nuclear reactions to the incident particle energy, taking deceleration into account. These relations are suitable for the design and assessment of pulsed neutron sources employing (p,n) reactions. Yield calculations for LiF are consistent with previous studies using explicit numerical integration of a proton spectrum through a target, and predict that the maximum neutron yield possible is around 0.25% of the incident protons. The yield from protons up to an incident energy of 35 MeV, 0.2%, is based on experimental measurements of the (p,n) cross-sections; the cross-section at higher energies was extrapolated and therefore uncertain in detail. The yield-energy curves will allow more direct optimization of configurations for the laser acceleration of protons to be used in pulsed neutro sources.

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